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Understanding molecular recognition and epitope prediction from Information Theoretic approach

Indranil Mitra[1*], Yan Cui[2]

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Background

Cellular immunity is dependent on T-cell recognition of peptide/major histocompatibility complex (MHC) and is a critical molecular recognition component [1]. A large class of bioinformatics tools facilitates the identification of T-cell epitopes to specific MHC alleles. However, not all peptide residues contribute equally or are relevant to binding due to polymorphism of genes encoding MHC, making development of statistical methods difficult. Information Theory has proved to be one of the most universal mathematical theories that governs virtually all processes [2]. The success of this approach in analyzing a huge range of engineering, technological and natural processes is impressive. In Molecular Biology the applications have been very successful at the sequence level, many sequence comparison and binding site identification methods now boasts a sound information theoretic foundation.

Materials and methods

In this work we have developed a mathematical formalism for applying information theory in identifying an explicit computational strategy and developing algorithms for the study of peptide/MHC interactions through epitope predictions. A sampling method has been initiated to circumvent the binding problem. Comparisons have been made with existing Machine Learning Methods and a validation of the efficiency of the model may be tested [3,4].The results will have significant impact for understanding the immune system and for rational drug design [5].

* Correspondence: aimitra@clemson.edu
[1]Department of Mathematical Sciences, Clemson University, E-006 Martin Hall, Clemson, SC 29631, USA

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Author details

[1]Department of Mathematical Sciences, Clemson University, E-006 Martin Hall, Clemson, SC 29631, USA. [2]Department of Molecular Sciences & Center of Integrative and Translational Genomics, University of Tennessee Health Science Center, 858 Madison Ave. Memphis, TN 38163, USA.

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